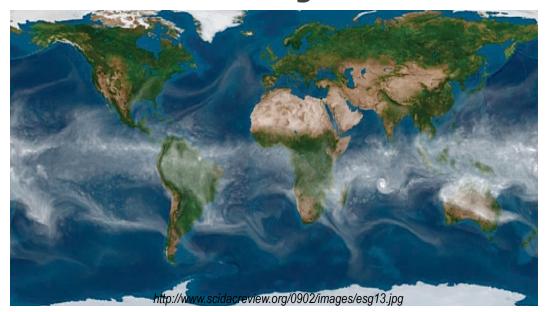
Porting The Spectral Element Community Atmosphere Model (CAM-SE) To Hybrid GPU Platforms



Matthew Norman

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Ilene Carpenter

Paulius Micikevicius

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2012 Programming weather, climate, and earth-system models on heterogeneous multi-core platforms





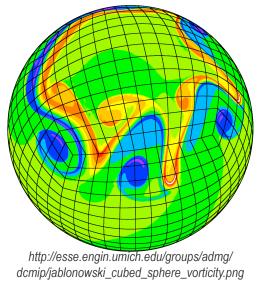
What is CAM-SE?

- Climate-scale atmospheric simulation for capability computing
- Comprised of (1) a dynamical core and (2) physics packages



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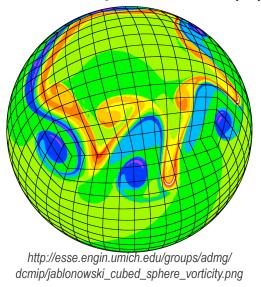
Dynamical Core

- "Dynamics": wind, energy, & mass
- "Tracer" Transport: $(H_2O, CO_2, O_3, ...)$ Transport quantities not advanced by the dynamics



What is CAM-SE?

- Climate-scale atmospheric simulation for capability computing
- Comprised of (1) a dynamical core and (2) physics packages

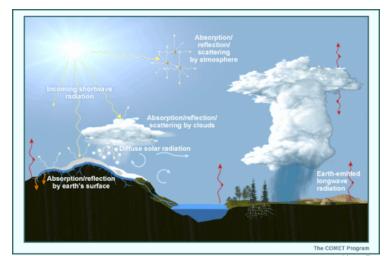


Dynamical Core

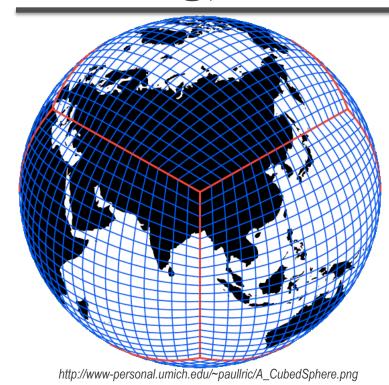
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 Transport quantities not advanced by the dynamics

Physics Packages

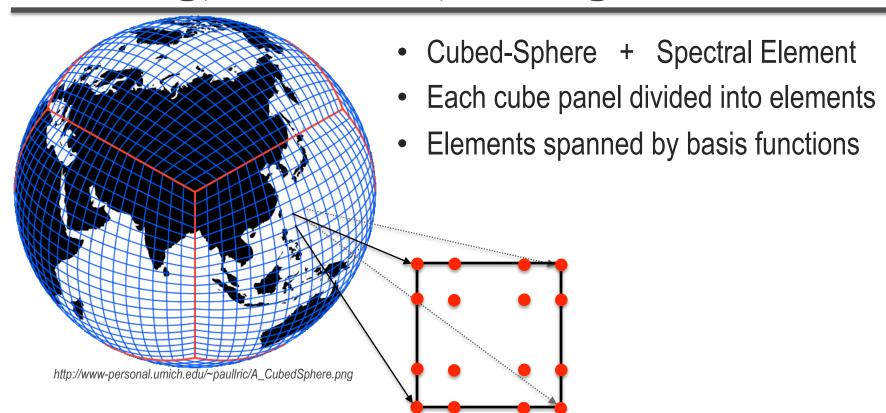
Resolve anything interesting not included in dynamical core (moist convection, radiation, chemistry, etc)

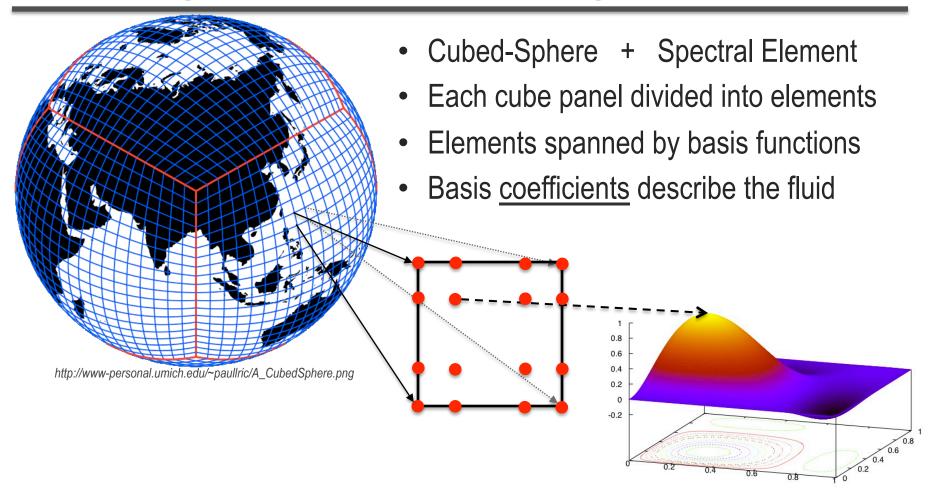


http://web.me.com/macweather/blogger/maweather_files/physprc2/gif

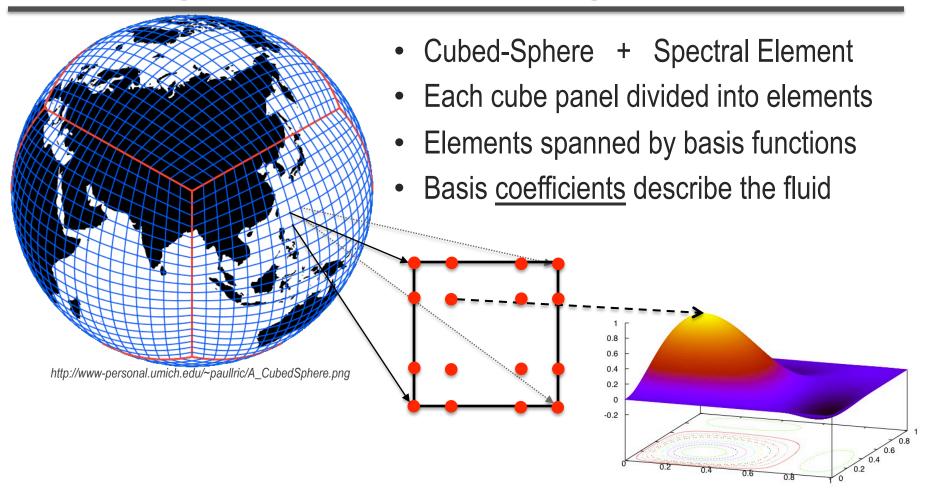


- Cubed-Sphere + Spectral Element
- Each cube panel divided into elements









Used CUDA FORTRAN from PGI

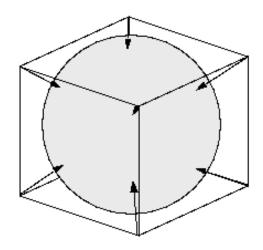
OACC Directives: Better software engineering option moving forward



16 billion degrees of freedom

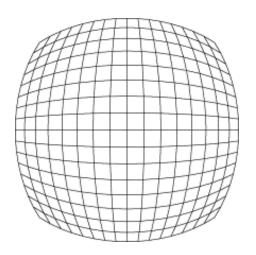


- 16 billion degrees of freedom
 - 6 cube panels



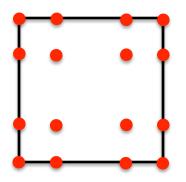


- 16 billion degrees of freedom
 - 6 cube panels
 - 240 x 240 columns of elements per panel

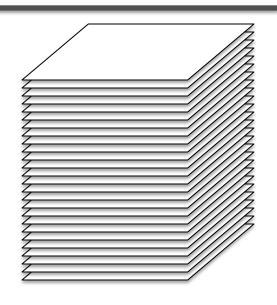




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$$H_2O$$
 , CO_2 , O_3 , CH_4 , ...

110 prognostic variables



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- Scaled to 14,400 XT5 nodes with 60% parallel efficiency



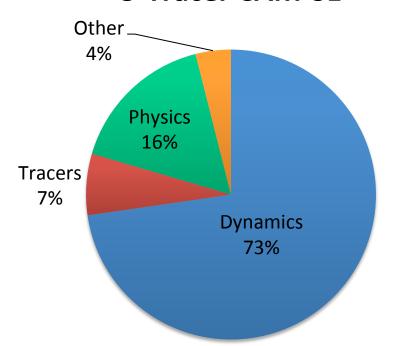
- 16 billion degrees of freedom
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 - 110 prognostic variables
- Scaled to 14,400 XT5 nodes with 60% parallel efficiency
- Must simulate 1-2 thousand times faster than real time
- With 10 second CAM-SE time step, need ≤ 10 ms per time step
 - 32-64 columns of elements per node, 5-10 thousand nodes



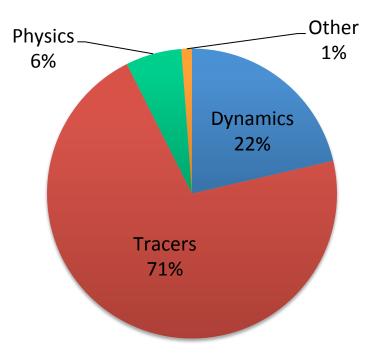
CAM-SE Profile (Cray XT5, 14K Nodes)

- Original CAM-SE used 3 tracers (20% difficult to port)
- Mozart chemistry provides 106 tracers (7% difficult to port)
 - Centralizes port to tracers with mostly data-parallel routines



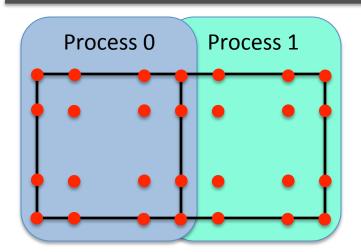


106-Tracer CAM-SE



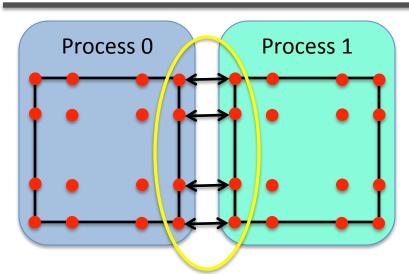


Communication Between Elements





Communication Between Elements

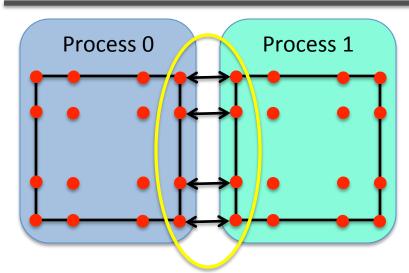


Physically occupy the same location, Spectral Element requires them to be equal

Edges are averaged, and the average replaces both edges



Communication Between Elements



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Edges are averaged, and the average replaces both edges

Implementation

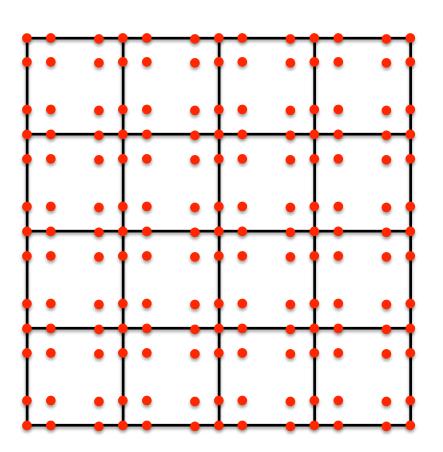
Edge_pack: pack <u>all</u> element edges into process-wide buffer. Data sent over MPI are contiguous in buffer.

Bndry_exchange: Send & receive data at domain decomposition boundaries

Edge_unpack: Perform a weighted sum for data at <u>all</u> element edges.



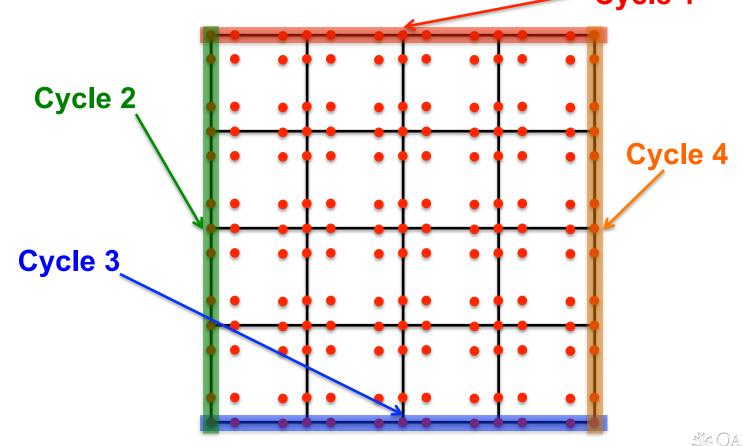
- Edge_pack ensures data for MPI is contiguous in buffer
- MPI communication occurs in "cycles"



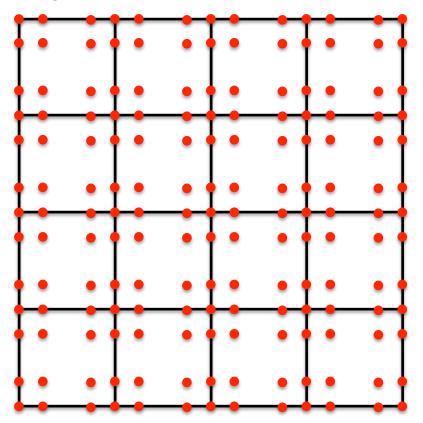


- Edge_pack ensures data for MPI is contiguous in buffer
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A cycle contains a contiguous data region for MPI Cycle 1

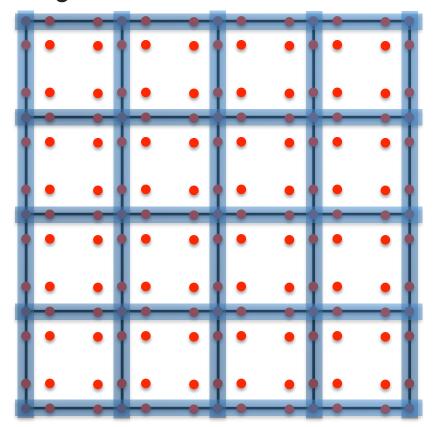


- Edge_pack ensures data for MPI is contiguous in buffer
- MPI communication occurs in "cycles"
- A cycle contains a contiguous data region for MPI
- Original pack/exchange/unpack



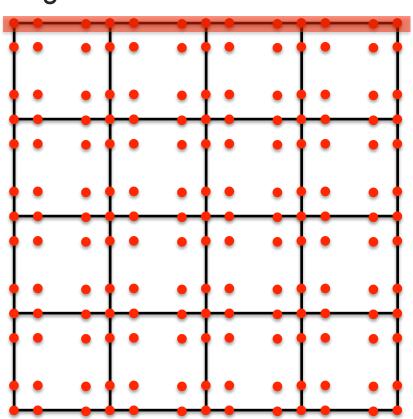


- Edge_pack ensures data for MPI is contiguous in buffer
- MPI communication occurs in "cycles"
- A cycle contains a contiguous data region for MPI
- Original pack/exchange/unpack
 - Pack all edges in a GPU Kernel



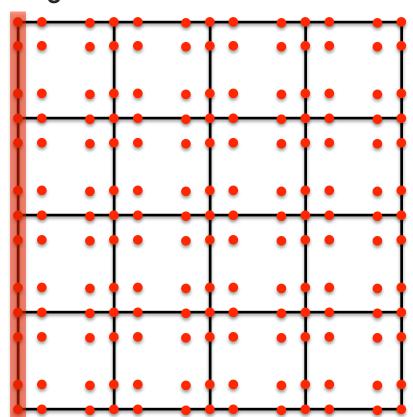


- Edge_pack ensures data for MPI is contiguous in buffer
- MPI communication occurs in "cycles"
- A cycle contains a contiguous data region for MPI
- Original pack/exchange/unpack
 - Pack all edges in a GPU Kernel
 - For each "send cycle"
 - Send cycle over PCI-e (D2H)
 - MPI_Isend the cycle



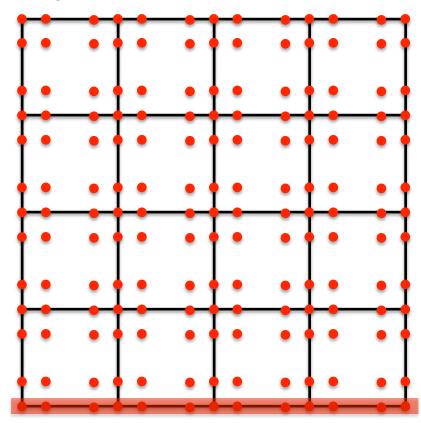


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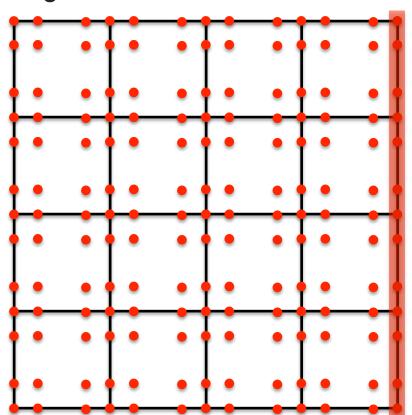


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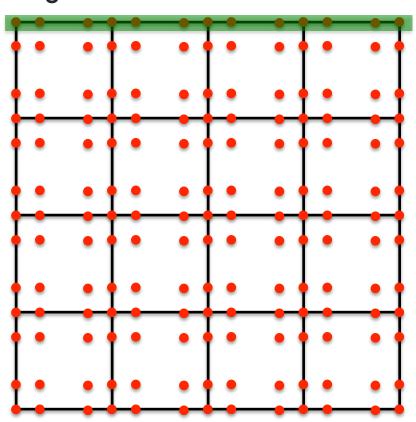


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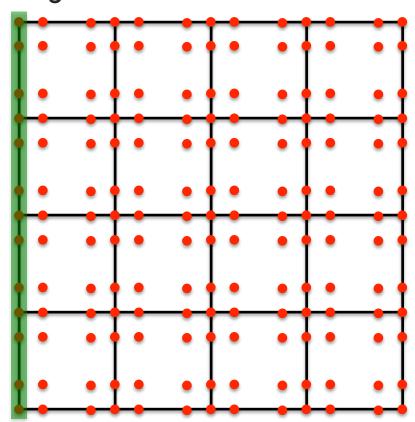


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 - MPI_Isend the cycle
 - For each "receive cycle"
 - MPI_Wait for the data
 - Send cycle over PCI-e (H2D)



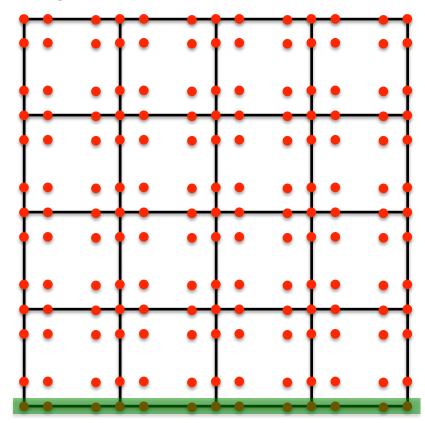


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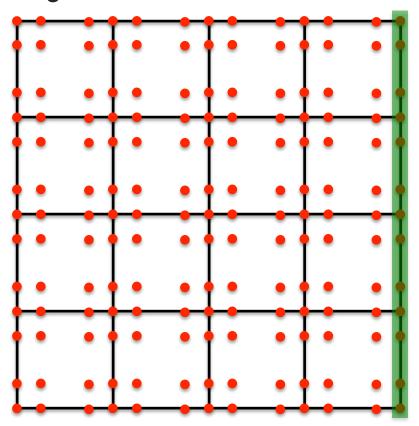


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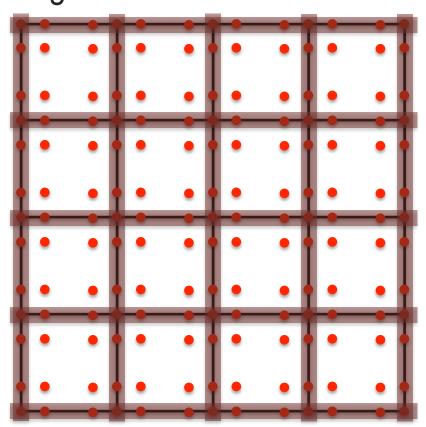


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 - For each "receive cycle"
 - MPI_Wait for the data
 - Send cycle over PCI-e (H2D)
 - Unpack all edges in a GPU Kernel





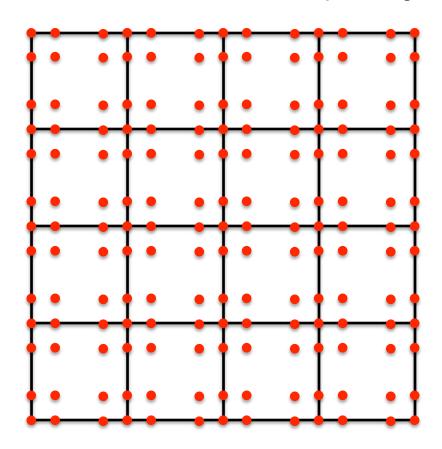
Optimizing Pack/Exchange/Unpack

- For a cycle, PCI-e D2H depends only on packing that cycle
 - <u>Divide</u> edge_pack into equal-sized cycles
 - 1. Find only the elements directly involved in each separate cycle
 - 2. Evenly divide remaining elements among the cycles
 - Associate each cycle with a unique CUDA stream
 - Launch each pack in its stream
 - After a cycle is packed, call async. PCI-e D2H in its Stream
- Edge_unpack at MPI boundaries requires all MPI to be finished
- However, internal unpacks can be done directly after packing



Porting Strategy: Pack/Exchange/Unpack

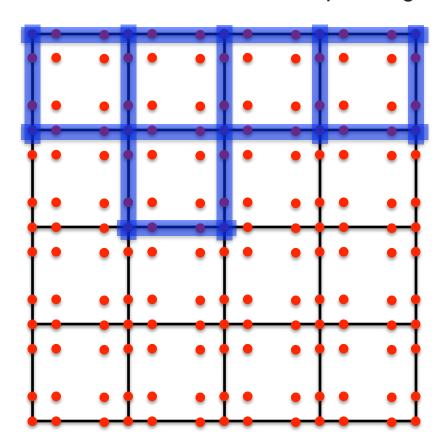
- For each cycle
 - Launch edge_pack kernel for the cycle in a unique stream
 - Call a cudaEventRecord for the stream's packing event





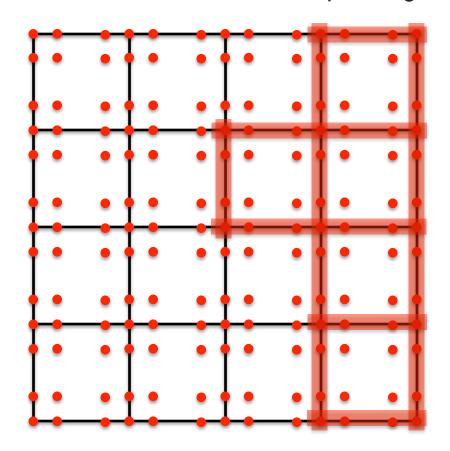
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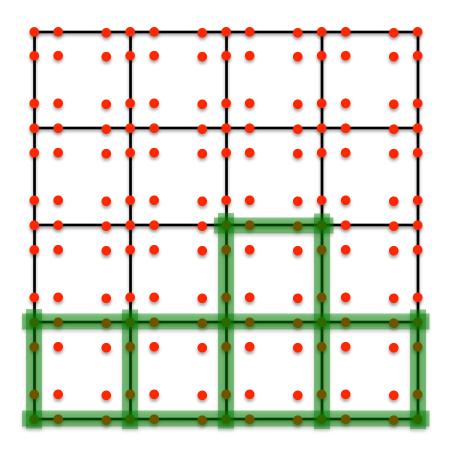


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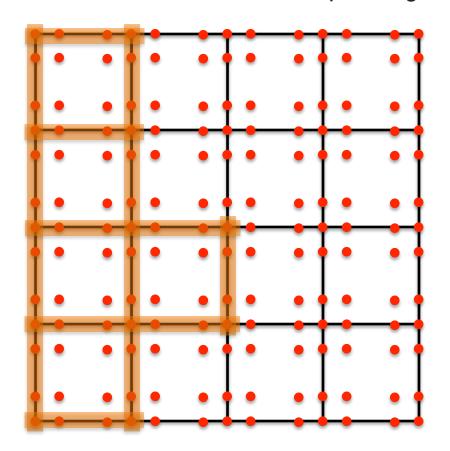


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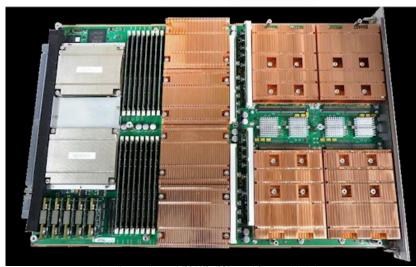
- For each cycle
 - Launch edge_pack kernel for the cycle in a unique stream
 - Call a cudaEventRecord for the stream's packing event



- Prepost each cycle's MPI_irecv
- While an MPI message remains pending
 - If <u>all</u> cycles finished packing (cudaEventQuery for all cycles' pack)
 - Launch edge_unpack kernel over elements not dealing with MPI
 - For each cycle
 - If cycle finished packing (cudaEventQuery for the cycle's pack)
 - Call async. PCI-e D2H copy for the cycle's MPI data
 - Call cudaEventRecord for a PCI-e D2H event
 - If cycle finished D2H PCI-e (cudaEventQuery for the cycle's D2H)
 - Call MPI_Isend for the cycle's MPI data
 - If MPI data has been received (MPI_Test for the cycle's transfer)
 - Call PCI-e H2D copy for the cycle's MPI data
- Call a device-wide barrier to ensure PCI-e H2D copies are done
- Unpack elements dealing with MPI





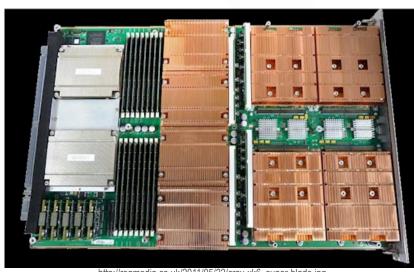


http://regmedia.co.uk/2011/05/22/cray-xk6_super-blade.jpg



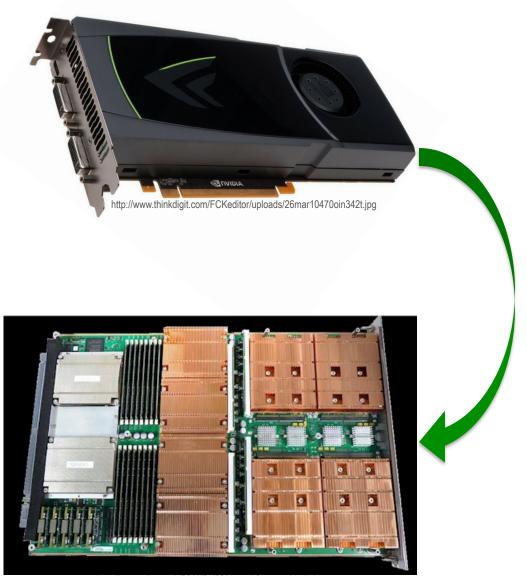


GPU Kernels



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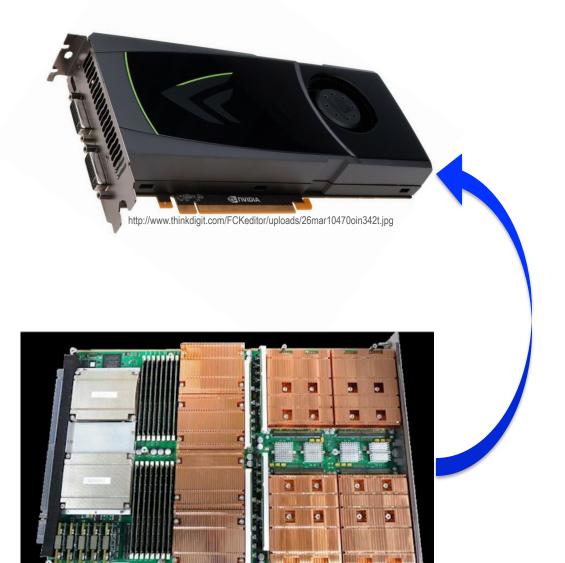


GPU Kernels

PCI-e D2H



http://regmedia.co.uk/2011/05/22/cray-xk6_super-blade.jpg



GPU Kernels

PCI-e D2H

PCI-e H2D



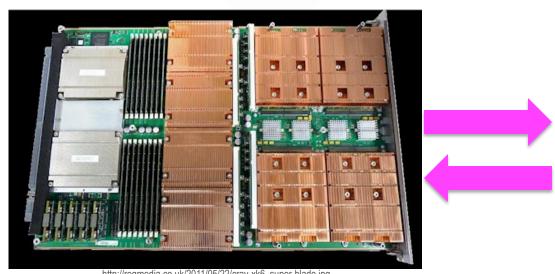


GPU Kernels

PCI-e D2H

PCI-e H2D

MPI











GPU Kernels

PCI-e D2H

PCI-e H2D

MPI

Host Computation



Other Important Porting Considerations

- Memory coalescing in kernels
 - Know how threads are accessing GPU DRAM, rethread if necessary
- Use of shared memory
 - Load data from DRAM to shared memory (coallesced)
 - Reuse as often as possible before re-accessing DRAM
 - Watch out for banking conflicts
- Overlapping kernels, CPU, PCI-e, & MPI
 - Perform independent CPU code during GPU kernels, PCI-e, & MPI
 - Break up & stage computations to overlap PCI-e, MPI, & GPU kernels
- PCI-e copies: consolidate if small, break up & pipeline if large
- GPU's user-managed cache made memory optimizations that are more difficult on a non-managed cache



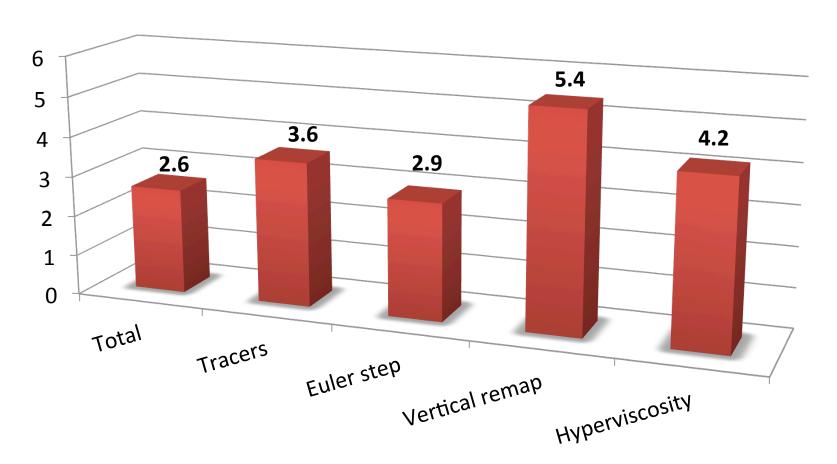
Usefulness Of Porting To Accelerators

- You understand your code's challenges for many threads
- You will often refactor the algorithms themselves
 - Vertical remap: splines + summation → PPM + two integrations
 - More flops, but more independence and less data movement
- You will change the way you thread
 - Higher-level hoisting of OpenMP to allow more parallelism
 - More data-independent work, more flops
 - Better staging through cache, less data in cache (less thrashing)
- Incorporating changes into CPU code almost always speeds up the CPU code
 - This changes perspective on code refactoring cost-benefit



Speed-Up: Fermi GPU vs 1 Interlagos / Node

- Benchmarks performed on XK6 using end-to-end wall timers
- All PCI-e and MPI communication included





Questions?

